

# AN INTERESTING CLASS OF PARTIAL DIFFERENTIAL EQUATIONS

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**ABSTRACT.** This paper presents an observation that under reasonable conditions, many partial differential equations from mathematical physics possess three structural properties. One of them can be understood as a variant of the celebrated Onsager reciprocal relation in Modern Thermodynamics. It displays a direct relation of irreversible processes to the entropy change. We show that the properties imply various entropy dissipation conditions for hyperbolic relaxation problems. As an application of the observation, we propose an approximation method to solve relaxation problems. Moreover, the observation is interpreted physically and verified with eight (sets of) systems from different fields.

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## 1. INTRODUCTION

The goal of this paper is to draw attention to a class of partial differential equations (PDEs) of the form

$$(1.1) \quad U_t + \sum_{j=1}^d F_j(U)_{x_j} = Q(U).$$

Here  $U$  is the unknown  $n$ -vector-valued function of  $(x, t) \equiv (x_1, x_2, \dots, x_d, t) \in \mathbf{R}^d \times [0, +\infty)$ , taking values in an open subset  $G$  of  $\mathbf{R}^n$  (called *state space*);  $Q(U)$  and  $F_j(U)$  ( $j = 1, 2, \dots, d$ ) are given  $n$ -vector-valued smooth functions of  $U \in G$ ; and the subscripts  $t$  and  $x_j$  refer to the partial derivatives with respect to  $t$  and  $x_j$ , respectively.

As fundamental PDEs and as intermediate models [7, 15, 19] between the Boltzmann equation [2] and hyperbolic conservation laws [4], systems of first-order PDEs with source terms describe various irreversible processes of scalar type [11]. Important examples occur

in chemically reactive flows [9], radiation hydrodynamics [17, 22], inviscid gas dynamics with relaxation [31], nonlinear optics [12], and so on.

Since the last decade, PDEs of the form (1.1) have attracted much attention. See [20, 28, 25] and references cited therein. One of the main interests is to identify a set of structural properties (axioms) that are satisfied by most of important equations from applications and, meanwhile, provide a convenient framework for the development of mathematical theories. In this regard, two stability conditions and various entropy dissipation conditions have been proposed in [26] and [3, 19, 29, 13, 25], respectively. See also [28, 23]. All those conditions are generalizations of the well-known subcharacteristic condition [16] for (1.1) with  $n = 2$  and  $d = 1$ . For (1.1), such a condition is the same in spirit as the H-theorem for the Boltzmann equation [2] and as the entropy condition for conservation laws [4].

In this paper, we present an observation that under reasonable assumptions, many equations of the form (1.1) from mathematical physics fall within a class characterized with the following three properties. (I) Every system in the class admits a strictly convex entropy function [10, 6], (II) the source term can be written as a product of a non-positive symmetric matrix and the corresponding entropy variable, and (III) the symmetric matrix has a constant null-space.

The first property is the well-known entropy condition for conservation laws and corresponds to the classical principles of thermodynamics. Property (II) can be understood as a variant of the celebrated Onsager reciprocal relation in Modern Thermodynamics [11, 14] and implies the second law of thermodynamics. It displays a direct relation of irreversible processes to the entropy change. Property (III) expresses the fact that physical laws of conservation hold true, no matter what state the underlying thermodynamical system is in (equilibrium, non-equilibrium, and so on).

We will verify the three properties for eight (sets of) systems of the form (1.1) arising in gas dynamics with damping or with relaxation, nonlinear optics, radiation hydrodynamics, chemical reactions, kinetic theories (both moment closure systems and discrete velocity models), and so on. Furthermore, we show that the properties ensure a uniquely defined Maxwellian and imply various entropy dissipation conditions in the literature for hyperbolic relaxation problems. Thus, all the general results in [27, 30, 18, 23, 29, 13, 25, 5] apply to the aforementioned fields.

We notice that the examples in Sections 8 and 9 have a common kinetic origin. Moreover, we know from [8] that the chemical systems in Section 7 have a similar origin. It would be interesting to include the radiative gas example of Section 6 in the same basket, with the idea that radiation is associated with particles (photons) collisions. In other words, we show that the kinetic theory yields the Onsager relation for gas mixtures.

As an application of our observation, we propose an approximation method to solve the relaxation problems. The accuracy of the method is analysed for initial value problems with smooth initial data, by using the results in [27]. In this analysis, an important ingredient is a continuation principle for hyperbolic singular limit problems (Lemma 9.1 in [28] and the appendix in [1]). Further analysis and applications of the approximation method are desirable.

Our discussions indicate that the above three properties have a solid basis, from both mathematical and physical points of view. Thus, it seems reasonable to take the properties as requirements in construction of new mathematical models for irreversible phenomena.

The paper is organized as follows. In Section 2 we present the observation and discuss its mathematical consequences. Section 3 is devoted to the approximation method. Some physical interpretations are given in Section 4. The rest of the paper deals with the eight (sets of) examples.

## 2. AN OBSERVATION

The main contribution of this paper is the following observation that under reasonable assumptions, many partial differential equations (PDEs) of the form (1.1) arising in mathematical physics admit the following structure:

(I). There is a strictly convex smooth function  $\eta(U)$  such that  $\eta_{UU}(U)F_{jU}(U)$  is symmetric for all  $U \in G$  and all  $j$ .

(II). There is a symmetric and non-negative definite matrix  $\mathcal{L} = \mathcal{L}(U)$  such that

$$Q(U) = -\mathcal{L}(U)\eta_U(U).$$

(III). The null space of  $\mathcal{L}(U)$  is independent of  $U \in G$ .

Throughout this paper,  $\eta_U(U)$  should be understood as a column vector. We will use  $*$  as a superscript to denote the transpose operator.

Recall that (I) is the classical observation due to Godunov [10], and Friedrichs and Lax [6] for conservation laws

$$U_t + \sum_{j=1}^d F_j(U)_{x_j} = 0.$$

In what follows, we point out several important conclusions of the above observation. First of all, we show

**Proposition 2.1.** *The observation is invariant under linear transformations of the form*

$$V = PU.$$

Here  $P$  is a constant and invertible  $n \times n$ -matrix.

*Proof.* Let  $\eta = \eta(U)$  be the strictly convex function in the observation. We need to show that the observation holds true with  $\tilde{\eta}(V) = \eta(P^{-1}V)$  for

$$(2.1) \quad V_t + \sum_j (PF_j(P^{-1}V))_{x_j} = PQ(P^{-1}V).$$

To this end, we compute

$$\eta_U = P^* \tilde{\eta}_V \quad \text{and} \quad \eta_{UU} = P^* \tilde{\eta}_{VV} P.$$

The second equality indicates that  $\tilde{\eta}_{VV}(V)$  is positive definite, since so is  $\eta_{UU}(U)$ . The latter is equivalent to the strict convexity of  $\eta(U)$ . Therefore,  $\tilde{\eta}(V)$  is strictly convex. Since

$$\tilde{\eta}_{VV}(PF_j(P^{-1}V))_V = (P^{-*} \eta_{UU} P^{-1})(PF_{jU} P^{-1}) = P^{-*} \eta_{UU} F_{jU} P^{-1}$$

is symmetric, (I) follows. Moreover, since

$$PQ(P^{-1}V) = -P\mathcal{L}\eta_U = -P\mathcal{L}P^* \tilde{\eta}_V$$

and  $P$  is independent of  $U$ , (II) and (III) follow. This completes the proof.  $\square$

Let  $r$  be such a constant that  $(n - r)$  is the dimension of the null space in (III). In Proposition 2.1, we take  $P$  to be such a matrix that its first  $(n - r)$  rows span the null space. Then the next proposition becomes obvious.

**Proposition 2.2.** *Under the observation, there is a constant invertible matrix  $P$  and a symmetric positive definite  $r \times r$ -matrix  $l(U)$  such that*

$$P\mathcal{L}(U)P^* = \text{diag}(0_{(n-r) \times (n-r)}, l(U)).$$

Here and below we denote by  $0_X$  the origin of  $\mathbf{R}^X$  to avoid possible confusions.

With  $P$  from Proposition 2.2, the source term in (2.1) obviously has the form

$$PQ(P^{-1}V) = \begin{pmatrix} 0_{n-r} \\ q(V) \end{pmatrix}$$

with  $q(V) \in \mathbf{R}^r$ . Accordingly, we introduce the partition

$$V = \begin{pmatrix} u \\ v \end{pmatrix}$$

and rewrite (2.1) as

$$(2.2) \quad \begin{pmatrix} u \\ v \end{pmatrix}_t + \sum_{j=1}^d \begin{pmatrix} f_j(u, v) \\ g_j(u, v) \end{pmatrix}_{x_j} = \begin{pmatrix} 0_{n-r} \\ q(u, v) \end{pmatrix}.$$

Notice that

$$(2.3) \quad q(u, v) = -l(u, v)\tilde{\eta}_v(u, v).$$

Because  $P$  is invertible and constant, (2.2) with (2.3) is equivalent to (1.1). Thus, one may assume that (1.1) is already in the form (2.2) with (2.3). In particular, the symmetric matrix  $\mathcal{L}$  in (II) has the block-diagonal form in Proposition 2.2 and  $l(U)$  therein is symmetric and positive definite.

With the equivalent form (2.2), we turn to the following theorem, which is related to the so-called equilibrium manifold

$$\mathcal{E} := \{U \in G : Q(U) = 0\}.$$

**Theorem 2.3.** *Assume that (1.1) possess the three observed properties and the state space  $G$  is convex. Then for every  $U \in G$ , there is at most one point in  $\mathcal{E}$ , say  $M = M(U)$ , such that  $U - M(U)$  is in the orthogonal complement of the null space. Moreover, there are two positive functions  $c(U) < C(U)$ , defined in the domain of  $M = M(U)$ , such that*

$$(2.4) \quad c(U)|U - M(U)| \leq |Q(U)| \leq C(U)|U - M(U)|.$$

Here  $|X|$  denotes the Euclid norm of matrix or vector  $X$ .

Note that  $M(U)$  may be defined only in part of the state space. A prototype of  $M(U)$  is the Maxwellian in kinetic theory [2].

*Proof.* Assume that for a certain  $U \in G$ , there are two points  $M_1, M_2 \in \mathcal{E}$  such that both  $U - M_1$  and  $U - M_2$  are in the orthogonal complement of the null space. Let  $P$  be the invertible matrix in Proposition 2.2 and set

$$PU = (u, v), \quad PM_1 = (u_1, v_1), \quad PM_2 = (u_2, v_2).$$

Then we have  $q(u_1, v_1) = 0 = q(u_2, v_2)$  and  $u_1 = u = u_2$ . Since  $l(u, v)$  is positive definite, from (2.3) it follows that  $q(u, v) = 0$  if and only if  $\tilde{\eta}_v(u, v) = 0$ . Thus we have  $\tilde{\eta}_v(u, v_1) = 0 = \tilde{\eta}_v(u, v_2)$ . This contradicts the strict convexity of  $\tilde{\eta}$  and thereby proves the first part of the theorem.

For the inequalities in (2.4), we denote by  $m(U)$  the last  $r$  components of  $M(U)$ . Since  $\tilde{\eta} = \tilde{\eta}(U)$  is strictly convex, there is a symmetric and positive definite  $r \times r$ -matrix  $a(U)$  such that

$$\tilde{\eta}_v(PU) = \tilde{\eta}_v(PU) - \tilde{\eta}_v(PM(U)) = a(U)(v - m(U)).$$

Thus, from (2.3) we have  $q(PU) = -l(PU)a(U)(v - m(U))$ . Now the inequalities in (2.4) can be easily verified with

$$\begin{aligned} c(U) &= (|P||P^{-1}||l^{-1}(PU)a^{-1}(U)|)^{-1}, \\ C(U) &= |P||P^{-1}||l(PU)a(U)|. \end{aligned}$$

This completes the proof.  $\square$

The following theorem provides connections of the observation to the existing entropy dissipation conditions in the literature for hyperbolic relaxation problems.

**Theorem 2.4.** *Assume that (1.1) possess the three observed properties. Then the following conclusions hold:*

- (1)  $\eta_U^*(U)Q(U) \leq -\lambda^{-1}(U)|Q(U)|^2$  for all  $U \in G$ , where  $\lambda(U)$  is the maximum eigenvalue of  $\mathcal{L}(U)$ .
- (2)  $Q(U) = 0$  if and only if  $\eta_U^*(U)Q(U) = 0$  if and only if  $\eta_U(U)$  is in the null space.
- (3)  $\eta_U^*(U_e)Q(U) = 0$  for any  $U, U_e \in G$  with  $U_e$  satisfying  $Q(U_e) = 0$ .
- (4) For  $U$  satisfying  $Q(U) = 0$ ,  $Q_U(U)\eta_{UU}^{-1}(U)$  is symmetric and non-positive definite, and its null space coincides with that of  $\mathcal{L}(U)$ .
- (5) For the equivalent version (2.2) with (2.3),  $r \times r$ -matrix  $q_v(u, v)$  is invertible for  $(u, v)$  satisfying  $q(u, v) = 0$ .

*Proof.* (1). Since  $\mathcal{L}(U)$  is symmetric and non-negative definite, it is clear that  $\mathcal{L}^2(U) \leq \lambda(U)\mathcal{L}(U)$ . Therefore we have

$$\eta_U^*(U)Q(U) = -\eta_U^*(U)\mathcal{L}(U)\eta_U(U) \leq -\lambda^{-1}|\mathcal{L}(U)\eta_U(U)|^2 = -\lambda^{-1}(U)|Q(U)|^2.$$

Note that the symmetry of  $\mathcal{L}(U)$  is crucial to the inequality.

(2). From (1) it follows immediately that  $Q(U) = 0$  if and only if  $\eta_U^*(U)Q(U) = 0$ . Since  $\eta_U^*(U)Q(U) = -\eta_U^*(U)\mathcal{L}(U)\eta_U(U)$  and  $\mathcal{L}(U)$  is symmetric,  $\eta_U^*(U)Q(U) = 0$  is obviously equivalent to that  $\eta_U(U)$  is in the null space of  $\mathcal{L}(U)$ .

(3). It follows from (II) that for  $U_e$  satisfying  $Q(U_e) = 0$ ,  $\eta_U(U_e)$  is in the null space of  $\mathcal{L}(U_e)$ . Thanks to (III),  $\eta_U(U_e)$  is in the null space of  $\mathcal{L}(U)$  for any  $U \in G$ . Thus, we have

$$(2.5) \quad \mathcal{L}(U)\eta_U(U_e) = 0$$

and thereby  $\eta_U^*(U_e)Q(U) = 0$  for any  $U, U_e \in G$  with  $U_e$  satisfying  $Q(U_e) = 0$ .

(4). From (II) and (2.5) it follows that

$$(2.6) \quad Q(U) = -\mathcal{L}(U)(\eta_U(U) - \eta_U(U_e)).$$

With this relation, it is clear that

$$Q_U(U_e) = -\mathcal{L}(U_e)\eta_{UU}(U_e).$$

Thus (4) becomes obvious.

(5). Recall the block-diagonal form of  $\mathcal{L}(u, v)$  for (2.2) with (2.3). It follows from (2) that  $\tilde{\eta}_v(u, v) = 0$  for  $(u, v)$  satisfying  $q(u, v) = 0$ . Thus, we compute from (2.3) that at  $(u, v)$  satisfying  $q(u, v) = 0$ ,  $q_v(u, v) = -l(u, v)\tilde{\eta}_{vv}(u, v)$ . Note that  $\tilde{\eta}_{vv}(u, v)$  is positive definite, since  $\tilde{\eta}(u, v)$  is strictly convex. This, together with the positive definiteness of  $l(u, v)$ , implies the invertibility of  $q_v(u, v)$ . Hence the proof is complete.  $\square$

By Theorem 2.4, if a system of PDEs possesses the three observed properties, then it satisfies all the entropy dissipation conditions in [3, 19, 29, 13, 25]. In fact, all the existing conditions consist of (I) and some additional requirements. They are  $\eta_U^*(U)Q(U) \leq 0$ , which is implied by (1) of Theorem 2.4, and (2) of Theorem 2.4 in [3]. In [19], there is only one additional requirement which is  $\eta_U^*(U)Q(U) \leq 0$  — the second law of thermodynamics. In [29], the additional requirements are (1) and (5) of Theorem 2.4, while they are (2) and (4) in [13]. The entropy dissipation condition in [25] is that in [29] with  $|Q(U)|$  in (1) replaced by  $|U - M(U)|$ . For this see the inequalities in (2.4). Moreover, it was shown in [29] that the entropy dissipation condition therein implies the stability conditions in [26, 27]. Thus, all the general results in [5, 13, 18, 23, 25, 27, 29, 30] are valid for PDEs of the form (1.1) which possess the three observed properties.

### 3. AN APPROXIMATION METHOD

Consider (1.1) with a small parameter  $\epsilon > 0$ :

$$(3.1) \quad U_t + \sum_j F_j(U)_{x_j} = Q(U)/\epsilon.$$

This is the so-called relaxation problem. Assume the three observed properties in the previous section hold for this relaxation system (3.1). Then the scaled system can be rewritten as

$$U_t + \sum_j F_j(U)_{x_j} = -\mathcal{L}(U)\eta_U(U)/\epsilon.$$

As an application of our observation, we show in this section that the above relaxation system can be approximated with the following simplified system

$$(3.2) \quad U_t + \sum_j F_j(U)_{x_j} = -\mathcal{L}(U_*)\eta_U(U)/\epsilon$$

as  $\epsilon$  tends to zero. Here  $U_* \in G$  is arbitrarily fixed.

To this end, we use the equivalent form (2.2):

$$(3.3) \quad \begin{pmatrix} u \\ v \end{pmatrix}_t + \sum_{j=1}^d \begin{pmatrix} f_j(u, v) \\ g_j(u, v) \end{pmatrix}_{x_j} = \frac{1}{\epsilon} \begin{pmatrix} 0_{n-r} \\ q(u, v) \end{pmatrix}.$$

Here

$$q(u, v) = -l(u, v)\tilde{\eta}_v(u, v)$$

as in (2.3). It is not difficult to see that as  $\epsilon$  goes to zero, the formal limit of solutions to (3.3) solves the following so-called equilibrium system

$$u_t + \sum_j f_j(u, v)_{x_j} = 0, \quad q(u, v) = 0.$$

This system consists of differential and algebraic equations.

Since  $q(u, v) = -l(u, v)\tilde{\eta}_v(u, v)$  and  $l(u, v)$  is positive definite, the equilibrium system is equivalent to

$$u_t + \sum_j f_j(u, v)_{x_j} = 0, \quad \tilde{\eta}_v(u, v) = 0.$$

This system is independent of  $l(u, v)$ . By Theorem 2.3, the algebraic equations define  $v$  as a unique function of  $u$ , say,  $v = h(u)$ . Here we assume that the domain of  $h(u)$  is non-empty and open! Thus, the equilibrium system becomes

$$(3.4) \quad u_t + \sum_j f_j(u, h(u))_{x_j} = 0, \quad v = h(u).$$

It is remarkable that  $h(u)$ , and thereby the equilibrium system, is independent of  $l(u, v)$ !

As is pointed out in the previous section, relaxation system (3.1) satisfies the stability conditions in [26, 27], for it possesses the three observed properties. Thus, Theorems 6.1 and 6.2 in [27] apply here: For smooth initial data, there is a finite and  $\epsilon$ -independent time interval  $[0, T]$  such that the initial value problem of (3.1) has a unique smooth solution  $U^\epsilon = U^\epsilon(x, t)$  defined for  $t \in [0, T]$  and satisfying

$$(3.5) \quad U^\epsilon = P^{-1} \begin{pmatrix} u \\ h(u) \end{pmatrix} + O(\epsilon)$$

in a certain Sobolev space, as  $\epsilon$  goes to zero. See [27] for details. Here  $u$  solves the corresponding initial value problem of the equilibrium system in (3.4). In addition, we have assumed for simplicity that the initial data take values in equilibrium and thereby initial-layers do not appear. Recall from [27] that the time interval  $[0, T]$  is the life-span of the smooth solution  $u$ .

Note that (3.4) is also the equilibrium system for the corresponding equivalent version (2.2) of the simplified system (3.2). The latter obviously possesses the three observed properties. Thus, we see that with the same initial data, the simplified system has a unique smooth solution  $\hat{U}^\epsilon$  defined in the same time interval and having the same expansion

$$(3.6) \quad \hat{U}^\epsilon = P^{-1} \begin{pmatrix} u \\ h(u) \end{pmatrix} + O(\epsilon)$$

as  $\epsilon$  goes to zero. Here the key points are the same equilibrium system and the same time interval. The latter is attributed to a continuation principle for hyperbolic singular limit problems (Lemma 9.1 in [28], see also the appendix in [1]). Consequently, we see from (3.5) and (3.6) that

$$U^\epsilon - \hat{U}^\epsilon = O(\epsilon),$$

in a certain Sobolev space, as  $\epsilon$  goes to zero.

In conclusion, we have shown that for small  $\epsilon$ , relaxation systems (3.1) and (3.2) are close to each other in a finite and  $\epsilon$ -independent time interval for initial value problems with smooth data. The above discussion suggests an approximation method to solve the original relaxation system (3.1). Further analysis and applications of this approximation method are desirable. In particular, it would be interesting to study the closeness for specific systems in the regime of non-smooth solutions.

#### 4. PHYSICAL INTERPRETATIONS

In this section, we give some physical interpretations of the three observed properties in Section 2. Recall that for a thermodynamic system inside which  $n$  irreversible processes occur, the infinitesimal entropy change  $dS$  due to the processes can be expressed as a sum of two parts:

$$dS = d_e S + d_i S.$$

Here  $d_e S$  is the part supplied to the system by its surroundings, and  $d_i S$  is that produced inside the system. It is well known (see, e.g., [11]) that  $d_e S$  corresponds to the flux terms in (1.1) and  $d_i S$  to the source term. The second law of thermodynamics states that  $d_i S$  is zero for reversible processes and positive for irreversible ones.

Based on our observation, (1.1) can be rewritten as

$$(4.1) \quad U_t + \sum_{j=1}^d F_j(U)_{x_j} = -\mathcal{L}(U)\eta_U(U).$$

This form relates irreversible processes directly to the entropy change  $\eta_U$ .

Recall that the physical entropy  $S$  is equal to  $-\eta$  and its existence is guaranteed by the classical principles of thermodynamics [11, 14]. This explains why the classical observation (I) has a solid basis in thermodynamics. The Gibbs relation on the total differential of  $\eta$  (or  $S$ ), in this general level, reads as

$$(4.2) \quad d\eta = \eta_U(U) \cdot dU,$$

where the dot “ $\cdot$ ” between two vectors means the scalar product. The usual Gibbs relation

$$\theta dS = de + pd\left(\frac{1}{\rho}\right) + \cdots$$

is a slight rearrangement of (4.2). Here  $\theta$  is the temperature,  $e$  is the specific internal energy,  $p$  is the pressure,  $\rho$  is the density, and the dots come from other possible internal variables.

Property (II) very much looks like the celebrated Onsager reciprocal relations in Non-equilibrium Thermodynamics [11, 14], if one understands the source terms as irreversible fluxes and the entropy variables as thermodynamic forces or affinities. However, it is slightly different from the Onsager relation. Firstly, it seems new to choose the entropy variables, instead of their linear combinations, as thermodynamic forces. Secondly, unlike the Onsager relation,

$$Q(U) = -\mathcal{L}(U)\eta_U(U)$$

is a nonlinear relation between  $Q(U)$  and  $\eta_U(U)$ . In fact, the matrix  $\mathcal{L} = \mathcal{L}(U)$  depends on  $U$ . Because the entropy function is strictly convex, there is a one-to-one correspondence



between  $U$  and the entropy variable  $\eta_U(U)$  (see [6] for a proof of this fact). Thus,  $\mathcal{L}$  depends on the entropy variable, which plays the role of affinities here.

By the way, it is well known (see, e.g., [21], page 125–126) that there are difficulties in choosing the thermodynamic forces and fluxes when applying the notion. Here we have proposed an unconventional but unambiguous choice of the couple.

Furthermore, we recall (2.6) and deduce that for any  $U, U_e \in G$  with  $U_e$  satisfying  $Q(U_e) = 0$ ,

$$\begin{aligned} Q(U) &= -\mathcal{L}(U)(\eta_U(U) - \eta_U(U_e)) \\ &= -\mathcal{L}(U_e)(\eta_U(U) - \eta_U(U_e)) - (\mathcal{L}(U) - \mathcal{L}(U_e))(\eta_U(U) - \eta_U(U_e)) \\ &= -\mathcal{L}(U_e)\eta_U(U) + O(|U - U_e|^2). \end{aligned}$$

Neglecting the higher-order term, we obtain a linear relation

$$Q(U) = -\mathcal{L}(U_e)\eta_U(U)$$

between  $Q(U)$  and  $\eta_U(U)$ . Because  $\mathcal{L}(U_e)$  is symmetric, this is the Onsager reciprocal relation if one considers the source terms as irreversible fluxes and the entropy variables as affinities.

As to Property (III), we recall the equivalent form (2.2) of (1.1). In (2.2), the first  $(n-r)$  equations represent  $(n-r)$  conservation laws. Note that  $r$  might not have been a constant without assuming (III). In other words, Property (III) expresses the fact that the physical laws of conservation hold true, no matter what state the underlying thermodynamical system is in (equilibrium, non-equilibrium, and so on).

## 5. FOUR SPECIFIC EXAMPLES

From this section on, we will verify the three observed properties in Section 2 for a number of systems of the form (1.1) arising in applications. This section contains four comparatively simple examples.

**Example 1.** Multi-dimensional Euler equations of gas dynamics with damping:

$$\begin{aligned} \rho_t + \operatorname{div}(\rho u) &= 0, \\ (\rho u)_t + \operatorname{div}(\rho u \otimes u) + \nabla p(\rho) &= -\rho u. \end{aligned}$$

As usual,  $\rho = \rho(x, t)$  stands for the density and  $u = u(x, t)$  is the velocity. This system is of the form (1.1) with  $U = \begin{pmatrix} \rho \\ \rho u \end{pmatrix} \in \mathbf{R}^{d+1}$ .

It is well known that function

$$\eta(U) = \frac{\rho|u|^2}{2} + \int^\rho \int^\tau \frac{p'(\sigma)}{\sigma} d\sigma d\tau.$$

is a strictly convex entropy for the above system in the classical sense (I). By computing  $\eta_U(U)$ , we see that

$$Q(U) = -\operatorname{diag}(0, \rho I_d)\eta_U(U),$$

where  $I_k$  is the unit matrix of order  $k$ . Thus, the properties (II) and (III) obviously hold with  $\mathcal{L}(U) = \operatorname{diag}(0, \rho I_d)$  for  $\rho > 0$ .

Next three examples all have the form (2.2) with  $r = 1$ . For such a system, if there is a function  $\eta = \eta(u, v)$  satisfying Property (I), then the observation is obviously true with

$$\mathcal{L}(U) = -\frac{q(u, v)}{\eta_v(u, v)} \text{diag}(0_{(n-r) \times (n-r)}, 1)$$

( $0_X$  is the origin of  $\mathbf{R}^X$ ), provided that

$$(5.1) \quad \frac{q(u, v)}{\eta_v(u, v)} < 0$$

for all  $(u, v)$  under consideration. The inequality (5.1) is a stability condition for the corresponding systems.

**Example 2.** A 3-D quasilinear system for nonlinear optics:

$$\begin{aligned} \vec{D}_t - \nabla \times \vec{B} &= 0, \\ \vec{B}_t + \nabla \times \vec{E} &= 0, \\ \chi_t &= |\vec{E}|^2 - \chi \end{aligned}$$

with  $\vec{D} = (1 + \chi)\vec{E}$ . See [12] for an explanation of the equations above. The state space here is  $G = \{(\vec{D}, \vec{B}, \chi) : \vec{D} \in \mathbf{R}^3, \vec{B} \in \mathbf{R}^3, \chi > 0\} \subset \mathbf{R}^7$ .

Set

$$U = \begin{pmatrix} \vec{D} \\ \vec{B} \\ \chi \end{pmatrix}.$$

In [12], Hanouzet and Huynh showed that function

$$\eta(U) \equiv (1 + \chi)^{-1} |\vec{D}|^2 + |\vec{B}|^2 + \chi^2/2$$

is a strictly convex entropy in the classical sense (I) in order to study the corresponding relaxation limit of the above system. By computing  $\eta_U(U)$ , we see that

$$Q(U) = -\text{diag}(0_{6 \times 6}, 1)\eta_U(U).$$

Thus, the observation is true with  $\mathcal{L}(U) = \text{diag}(0_{6 \times 6}, 1)$ .

**Example 3.** 1-D Euler equations of gas dynamics in vibrational non-equilibrium (in Lagrangian coordinates):

$$\begin{aligned} \nu_t - u_x &= 0, \\ u_t + p_x &= 0, \\ (e + \frac{u^2}{2})_t + (pu)_x &= 0, \\ q_t &= \omega(\theta_1) - \omega(\theta_2). \end{aligned}$$

See [31] for an explanation of the equations above.

For this system, we know from [31] that there is a strictly convex function  $\eta = \eta(\nu, u, e + \frac{u^2}{2}, q)$  such that Property (I) holds and

$$\eta_q(U) = \frac{1}{\theta_1} - \frac{1}{\theta_2}.$$

Then we have

$$Q(U) = -\theta_1\theta_2 \frac{\omega(\theta_1) - \omega(\theta_2)}{\theta_1 - \theta_2} \text{diag}(0_{3 \times 3}, 1) \eta_U(U).$$

Thus, the observation is true with

$$\mathcal{L}(U) = \theta_1\theta_2 \frac{\omega(\theta_1) - \omega(\theta_2)}{\theta_1 - \theta_2} \text{diag}(0_{3 \times 3}, 1),$$

for  $\omega = \omega(\theta)$  is strictly increasing [31].

**Example 4.** 1-D Euler equations for isothermal motions of a viscoelastic material (in Lagrangian coordinates):

$$\begin{aligned} \nu_t - u_x &= 0, \\ u_t + p_x &= 0, \\ (p + E\nu)_t &= -p - g(\nu). \end{aligned}$$

See [24] for an explanation of the equations above.

For this system, we know from [24] that function

$$\eta(U) = u^2/2 - E\nu^2/2 - p\nu - \int^{-p-E\nu} h^{-1}(\sigma) d\sigma,$$

is a strictly convex entropy in the classical sense (I). Here  $h^{-1}$  is the inverse of  $h(\nu) = g(\nu) - E\nu$ , which exists under the so-called subcharacteristic condition

$$(5.2) \quad 0 < g_\nu(\nu) < E.$$

Since

$$\eta_p(U) = h^{-1}(-p - E\nu) - \nu,$$

we have

$$Q(U) = -\frac{p + g(\nu)}{h^{-1}(-p - E\nu) - \nu} \text{diag}(0_{2 \times 2}, 1) \eta_U(U).$$

Thus, the observation is true with

$$\mathcal{L}(U) = \frac{p + g(\nu)}{h^{-1}(-p - E\nu) - h^{-1}(h(\nu))} \text{diag}(0_{2 \times 2}, 1),$$

for  $h(\nu) = g(\nu) - E\nu$  is strictly decreasing [24] under the subcharacteristic condition (5.2).

## 6. RADIATION HYDRODYNAMICS

In this section, we consider discrete-ordinate models of the Euler equations for radiation hydrodynamics [17, 22], which are of the form (1.1) with

$$U = \begin{pmatrix} \rho \\ \rho v_1 \\ \rho v_2 \\ \rho v_3 \\ \rho E \\ I_1 \\ \vdots \\ I_L \end{pmatrix}, \quad F_j(U) = \begin{pmatrix} \rho v_j \\ \rho v_1 v_j + \delta_{1j} p \\ \rho v_2 v_j + \delta_{2j} p \\ \rho v_3 v_j + \delta_{3j} p \\ \rho E v_j + p v_j \\ \mu_j^1 I_1 \\ \vdots \\ \mu_j^L I_L \end{pmatrix}, \quad Q(U) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ C \rho \sum_{l=1}^L (I_l - B(\theta)) \\ -\rho(I_1 - B(\theta)) \\ \vdots \\ -\rho(I_L - B(\theta)) \end{pmatrix}.$$

Here  $\rho$  is the density,  $v_j$  is the velocity in the  $j^{\text{th}}$  direction,  $E = e + |v|^2/2$  with  $e$  the specific internal energy,  $I_l$  is the radiation intensity in the direction  $\mu^l = (\mu_1^l, \mu_2^l, \mu_3^l)$ ,  $p = p(\rho, e)$  is the pressure,  $\delta_{ij}$  is the standard Kronecker delta,  $C$  is a positive constant, and  $B = B(\theta)$  is the Planck function of temperature  $\theta$ .

For this system, the state space is  $(0, \infty) \times \mathbf{R}^3 \times (0, \infty)^{L+1}$ . Since the basic assumptions of radiation hydrodynamics are not valid at low temperatures, we restrict the temperature domain to  $[\theta_0, \infty)$  with  $\theta_0 > 0$  a constant.

Recall that  $B = B(\theta) > 0$  is strictly increasing with respect to  $\theta \geq \theta_0$ . We denote by  $b = b(y)$  the inverse function of  $B(\theta)$ , that is,

$$(6.1) \quad \theta = b(B(\theta)), \quad \forall \theta \geq \theta_0.$$

Note that  $b = b(y)$  is strictly increasing. Moreover, it is smooth if so is  $B = B(\theta)$ .

Define

$$(6.2) \quad \eta(U) = -\rho s(\rho, e) - C \sum_{l=1}^L \int_{B(\theta_0)}^{I_l} \frac{dy}{b(y)}$$

with  $s = s(\rho, e)$  the specific entropy. It is straightforward to verify that this  $\eta$  is strictly convex. Since the system is the classical Euler equations coupled weakly to  $L$  linear transport equations,  $\eta$  is obviously an entropy function for the system. Namely, Property (I) is verified.

Note that

$$\eta_{\rho E}(U) = -\frac{1}{\theta}, \quad \eta_{I_l}(U) = -\frac{C}{b(I_l)}$$

and set

$$\sigma_l := \frac{I_l - B(\theta)}{\theta^{-1} - b^{-1}(I_l)}.$$

Then it is not difficult to see that

$$Q(U) = -\mathcal{L}(U)\eta_U(U)$$

with

$$(6.3) \quad \mathcal{L}(U) = \rho \begin{pmatrix} 0_{4 \times 4} & 0_{4 \times 1} & 0_{4 \times 1} & 0_{4 \times 1} & 0_{4 \times 1} & \cdots & 0_{4 \times 1} \\ 0_{1 \times 4} & C \sum_l \sigma_l & -\sigma_1 & -\sigma_2 & -\sigma_3 & \cdots & -\sigma_L \\ 0_{1 \times 4} & -\sigma_1 & C^{-1}\sigma_1 & 0 & 0 & \cdots & 0 \\ 0_{1 \times 4} & -\sigma_2 & 0 & C^{-1}\sigma_2 & 0 & \cdots & 0 \\ 0_{1 \times 4} & -\sigma_3 & 0 & 0 & C^{-1}\sigma_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0_{1 \times 4} & -\sigma_L & 0 & 0 & 0 & \cdots & C^{-1}\sigma_L \end{pmatrix}.$$

Since  $\sigma_l > 0$  for all  $l$ , this  $\mathcal{L}(U)$  is symmetric and non-negative. Moreover, its null space is

$$\text{span} \left\{ e_1, e_2, e_3, e_4, e_5 + C \sum_{l \geq 6} e_l \right\},$$

which is independent of  $U$ . Here  $e_k$  is the  $k^{\text{th}}$  column of the unit matrix  $I_{(L+5)}$ . Consequently, the properties (II) and (III) are also verified.

## 7. CHEMICALLY REACTIVE FLOWS

Most of this section is taken from [9], except the verification of the properties II and (III). For multi-component reactive flows, if we neglect external forces, diffusion of mass, heat conduction and viscosity, and but retain the chemical reactions, the flows are described with PDEs of form (1.1), where

$$(7.1) \quad U = \begin{pmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_{n_s} \\ \rho v_1 \\ \rho v_2 \\ \rho v_3 \\ \rho E \end{pmatrix}, \quad F_j(U) = \begin{pmatrix} \rho_1 v_j \\ \rho_2 v_j \\ \vdots \\ \rho_{n_s} v_j \\ \rho v_1 v_j + \delta_{1j} p \\ \rho v_2 v_j + \delta_{2j} p \\ \rho v_3 v_j + \delta_{3j} p \\ \rho E v_j + p v_j \end{pmatrix}, \quad Q(U) = \begin{pmatrix} m_1 \omega_1 \\ m_2 \omega_2 \\ \vdots \\ m_{n_s} \omega_{n_s} \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Here  $\rho_k$  is the density of the  $k^{\text{th}}$  species,  $n_s$  is the number of the species,  $\rho = \sum_k \rho_k$  is the total density,  $v_j$  is the mass averaged flow velocity in the  $j^{\text{th}}$  direction,  $E = e + |v|^2/2$  with  $e$  the specific internal energy of the mixture,  $p$  is the pressure,  $\delta_{ij}$  is the standard Kronecker delta,  $m_k$  is the molar mass of the  $k^{\text{th}}$  species (known constants), and  $\omega_k$  is the molar production rate of the  $k^{\text{th}}$  species. The system of will be closed by specifying  $e, p$  and  $\omega_k$  as functions of the natural variable

$$(7.2) \quad Y = (\rho_1, \rho_2, \dots, \rho_{n_s}, v_1, v_2, v_3, \theta)^*$$

with  $\theta$  the absolute temperature.

We will specify  $\omega_k$  later.  $p$  and  $e$  are given as in [9]. For  $p$ , we denote by  $R_g$  the universal gas constant, write  $r_k = R_g/m_k$  and then define

$$(7.3) \quad p = \theta \sum_k r_k \rho_k.$$

$e$  is taken as the weighted average of the specific internal energy  $\epsilon_k$  of the  $k^{th}$  species:

$$(7.4) \quad \rho e = \sum_k \rho_k \epsilon_k,$$

where

$$(7.5) \quad \epsilon_k = \epsilon_k^0 + \int_{\theta_0}^{\theta} c_{vk}(y) dy.$$

Here  $\epsilon_k^0$  is the specific internal energy of the  $k^{th}$  species at the reference temperature  $\theta_0 > 0$ , and  $c_{vk} = c_{vk}(\theta)$  are given smooth functions of  $\theta \in [\theta_0, \infty)$ , denoting the specific heat at constant volume of the  $k^{th}$  species and satisfying  $\min_{k,\theta} \{c_{vk}(\theta)\} > 0$ .

The state space for the natural variable  $Y$  defined in (7.2) is  $(0, \infty)^{n_s} \times \mathbf{R}^3 \times [\theta_0, \infty)$ . For the conserved variable  $U$  defined in (7.1), it is

$$G \equiv \{U \in \mathbf{R}^{n_s+4} : U_k > 0 \text{ for } 1 \leq k \leq n_s \text{ and } U_{n_s+4} > \phi(U_1, U_2, \dots, U_{n_s+3})\},$$

where

$$\phi(U_1, U_2, \dots, U_{n_s+3}) = \frac{U_{n_s+1}^2 + U_{n_s+2}^2 + U_{n_s+3}^2}{2 \sum_{k \leq n_s} U_k} + \sum_{k \leq n_s} U_k \epsilon_k^0.$$

Since  $\phi$  is a convex function, the state space  $G$  is convex.

Introduce

$$(7.6) \quad s_k(\rho_k, \theta) = s_k^0 + \int_{\theta_0}^{\theta} \frac{c_{vk}(y)}{y} dy - r_k \ln \left( \frac{\rho_k}{m_k} \right),$$

where  $s_k^0$  is a constant, and define

$$(7.7) \quad \eta(U) = - \sum_k \rho_k s_k(\rho_k, \theta).$$

We show that this  $\eta = \eta(U)$  is an entropy function in the classical sense (I). Since

$$\rho E = \sum_k \rho_k \left( \epsilon_k^0 + \int_{\theta_0}^{\theta} c_{vk}(y) dy \right) + \frac{\rho |v|^2}{2}$$

due to (7.4) and (7.5), we compute to obtain

$$\theta_U = \left( \sum_k \rho_k c_{vk}(\theta) \right)^{-1} \left( \frac{|v|^2}{2} - \epsilon_1, \dots, \frac{|v|^2}{2} - \epsilon_{n_s}, -v_1, -v_2, -v_3, 1 \right).$$

Thus, it follows from (7.7) and (7.6) that

$$(7.8) \quad \eta_U = \frac{1}{\theta} \left( \mu_1 - \frac{|v|^2}{2}, \dots, \mu_{n_s} - \frac{|v|^2}{2}, v_1, v_2, v_3, -1 \right)^*,$$

where

$$(7.9) \quad \mu_k = \epsilon_k + r_k \theta - s_k \theta$$

denotes the chemical potential of the  $k^{th}$  species. On the other hand, by the definitions of  $U$  and  $Y$  in (7.1) and (7.2), we compute

$$\frac{\partial Y}{\partial U} = \begin{pmatrix} I_{n_s} & 0_{n_s \times 3} & 0_{n_s \times 1} \\ -\rho^{-1}v(1, 1, \dots, 1) & \rho^{-1}I_3 & 0_{3 \times 1} \\ & \theta_U & \end{pmatrix}$$

with  $v = (v_1, v_2, v_3)^*$ , and thereby

$$\begin{aligned} \eta_{UU}(U) &= \frac{\partial \eta_U}{\partial U} = \frac{\partial \eta_U}{\partial Y} \frac{\partial Y}{\partial U} \\ &= \begin{pmatrix} (\delta_{kl} r_l \rho_k^{-1})_{n_s \times n_s} & -\theta^{-1}(1, 1, \dots, 1)^* v^* & \theta^{-2}(\frac{|v|^2}{2} - \epsilon_k) \\ 0_{3 \times n_s} & \theta^{-1}I_3 & -\theta^{-2}v \\ 0_{1 \times n_s} & 0_{1 \times 3} & \theta^{-2} \end{pmatrix} \frac{\partial Y}{\partial U} \\ &= \left( \frac{\partial Y}{\partial U} \right)^* \begin{pmatrix} (\delta_{kl} r_l \rho_k^{-1})_{n_s \times n_s} & 0_{n_s \times 3} & 0_{n_s \times 1} \\ 0_{3 \times n_s} & \rho \theta^{-1}I_3 & 0_{3 \times 1} \\ 0_{1 \times n_s} & 0_{1 \times 3} & \theta^{-2} \sum_k \rho_k c_{vk}(\theta) \end{pmatrix} \frac{\partial Y}{\partial U} > 0. \end{aligned}$$

Therefore,  $\eta(U)$  is strictly convex. Moreover, since

$$\sum_j \xi_j F_j(U) = (v \cdot \xi)U + \begin{pmatrix} 0_{n_s \times 1} \\ \xi \\ v \cdot \xi \end{pmatrix} p$$

due to (7.1), we have

$$\partial_U \left( \sum_j \xi_j F_j(U) \right) = (v \cdot \xi)I_{n_s+4} + \begin{pmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_{n_s} \\ \rho v \\ \rho E + p \end{pmatrix} \partial_U(v \cdot \xi) + \begin{pmatrix} 0_{n_s \times 1} \\ \xi \\ v \cdot \xi \end{pmatrix} p_U.$$

Therefore, it follows from (7.8), (7.3), (7.4), (7.9) and (7.7) that

$$\eta_U^* \partial_U \left( \sum_j \xi_j F_j(U) \right) = (v \cdot \xi) \eta_U^* + \eta \partial_U(v \cdot \xi) = \partial_U(v \cdot \xi \eta).$$

Hence,  $\eta(U)$  is a strictly convex entropy function for the system in the classical sense (I).

Next we turn to specifying  $\omega_k$  by following [9] again. Let the system have  $n_r$  reversible reactions for  $n_s$  species:

$$\sum_k \nu'_{ki} \mathcal{S}_k \rightleftharpoons \sum_k \nu''_{ki} \mathcal{S}_k$$

for  $i = 1, 2, \dots, n_r$ . Here  $\mathcal{S}_k$  is the chemical symbol for the  $k^{th}$  species, and  $\nu'_{ki}$  and  $\nu''_{ki}$  are the stoichiometric coefficients of the  $k^{th}$  species in the  $i^{th}$  reaction. The molar production rates  $\omega_k$  are the Maxwellian production rates obtained in the kinetic framework

of the “slow reaction regime” or in the “tempered reaction regime”, when the chemical charactersitic times are larger than the mean free times of molecules:

$$(7.10) \quad \omega \equiv (\omega_1, \omega_2, \dots, \omega_{n_s})^* = \sum_i \tau_i (\nu_{1i}, \nu_{2i}, \dots, \nu_{n_s i})^* \equiv \sum_i \tau_i \nu_i.$$

Here  $\nu_{ki} = \nu''_{ki} - \nu'_{ki}$  and  $\tau_i$  is the rate of progress of the  $i^{th}$  reaction:

$$(7.11) \quad \tau_i = K_{fi}(\theta) \prod_k \left( \frac{\rho_k}{m_k} \right)^{\nu'_{ki}} - K_{ri}(\theta) \prod_k \left( \frac{\rho_k}{m_k} \right)^{\nu''_{ki}},$$

where  $K_{fi}(\theta)$  and  $K_{ri}(\theta)$  are the direct and reverse constants of the  $i^{th}$  reaction, respectively; and

$$(7.12) \quad \frac{K_{fi}(\theta)}{K_{ri}(\theta)} = K_{ei}(\theta) := \exp \left( - \sum_k (r_k \theta)^{-1} \nu_{ki} \mu_k(m_k, \theta) \right)$$

with  $\mu_k(m_k, \theta)$  the chemical potential (7.9) at the unit concentration:  $\rho_k/m_k = 1$ .

It is well know that

$$\sum_k m_k \omega_k = 0.$$

In fact, let  $n_e$  be the number of elements involved in the system and denote by  $e_{kl}$  the number of the  $l^{th}$  element in the  $k^{th}$  species. We have the *element conservation* relations

$$(7.13) \quad \sum_k \nu'_{ki} \epsilon_{kl} = \sum_k \nu''_{ki} \epsilon_{kl}$$

for  $i = 1, 2, \dots, n_r$  and  $l = 1, 2, \dots, n_e$ . On the other hand, the species molar mass  $m_k$  is related to the elemental masses  $a_l$  by the relation

$$m_k = \sum_l a_l \epsilon_{kl}.$$

Hence it follows from (7.10) and (7.13) that

$$\sum_k m_k \omega_k = \sum_k \sum_{i,l} a_l \epsilon_{kl} \tau_i \nu_{ki} = \sum_{i,l} a_l \tau_i \sum_k \epsilon_{kl} (\nu''_{ki} - \nu'_{ki}) = 0.$$

Similarly, we have

$$(7.14) \quad \sum_k m_k \nu_{ki} = 0.$$

To see the properties (II) and (III), we set

$$M = \text{diag}(m_1, m_2, \dots, m_{n_s}), \quad \mathcal{Y} = (R_g \theta)^{-1} (\mu_1, \mu_2, \dots, \mu_{n_s})^*.$$

and

$$\Delta_i = K_{fi}(\theta) \prod_k \left( \frac{\rho_k}{m_k} \right)^{\nu'_{ki}} \int_0^1 \exp(\sigma \langle \mathcal{Y}, M \nu_i \rangle) d\sigma > 0.$$



It follows from (7.11), (7.12), (7.9), (7.6), (7.10) and (7.14) that

$$\begin{aligned}\tau_i &= -\Delta_i \nu_i^* M \mathcal{Y} \\ &= -(R_g \theta)^{-1} \Delta_i \nu_i^* M \left( \mu_1 - \frac{|v|^2}{2}, \mu_2 - \frac{|v|^2}{2}, \dots, \mu_{n_s} - \frac{|v|^2}{2} \right)^*.\end{aligned}$$

Note that the reaction rates  $\tau_i$  depend exponentially on the chemical affinities  $\nu_i^* M \mathcal{Y}$ , due to

$$\int_0^1 \exp(\sigma < \mathcal{Y}, M \nu_i >) d\sigma = \frac{\exp(< \mathcal{Y}, M \nu_i >) - 1}{\nu_i^* M \mathcal{Y}}.$$

Moreover, we set

$$V = (\nu_1, \nu_2, \dots, \nu_{n_r}) \quad \text{and} \quad \Delta = \text{diag}(\Delta_1, \Delta_2, \dots, \Delta_{n_r}).$$

Then we deduce from (7.1), (7.10) and (7.8) that

$$Q(U) = -R_g^{-1} \text{diag}(MV \Delta V^* M, 0_{4 \times 4}) \eta_U(U).$$

Since  $MV$  is a constant matrix and  $\Delta$  is positive definite, the null space of  $MV \Delta V^* M$  is independent of  $U$ . Hence the observation is verified with

$$\mathcal{L}(U) = R_g^{-1} \text{diag}(MV \Delta V^* M, 0_{4 \times 4}).$$

Finally, let us mention that some statements of Proposition 2.4 are also discussed in [9].

## 8. MOMENT CLOSURE SYSTEMS

Moment closure systems in kinetic theories are PDEs of the form (1.1). In this section we show that our observation holds for the exponentially based closure systems in [15] corresponding to the Boltzmann equation

$$(8.1) \quad f_t + \xi \cdot \nabla_x f = \int_{(\omega, \xi') \in S^{d-1} \times \mathbf{R}^d} (f_\star f'_\star - f f') B(\omega, \xi, \xi') d\omega d\xi'.$$

Here  $f = f(x, t, \xi) \geq 0$  denotes the kinetic density of particles at the position-time-velocity point  $(x, t, \xi) \in \mathbf{R}^d \times \mathbf{R}_+ \times \mathbf{R}^d$ , the dot “ $\cdot$ ” between two vectors means the scalar product,  $f_\star = f(x, t, \xi_\star)$ ,  $f'_\star = f(x, t, \xi'_\star)$  and  $f' = f(x, t, \xi')$  with

$$\xi_\star = \xi - \omega \cdot (\xi - \xi') \omega \quad \text{and} \quad \xi'_\star = \xi' + \omega \cdot (\xi - \xi') \omega,$$

$B = B(\omega, \xi, \xi')$  is the collision kernel which is positive almost everywhere in its domain  $S^{d-1} \times \mathbf{R}^d \times \mathbf{R}^d$ , and  $d\omega$  is the normalized measure on the unit sphere  $S^{d-1}$ .

First of all, we recall the celebrated identity (see [2])

$$(8.2) \quad 4 \int \phi(\xi) (f_\star f'_\star - f f') B d\omega d\xi' d\xi = \int (\phi + \phi' - \phi_\star - \phi'_\star) (f_\star f'_\star - f f') B d\omega d\xi' d\xi$$

for any continuous function  $\phi = \phi(\xi)$ . Here and below, the integrals are taken over the whole domain and we write  $\phi' = \phi(\xi')$ ,  $\phi_\star = \phi(\xi_\star)$  and  $\phi'_\star = \phi(\xi'_\star)$ . The identity is a direct result of the following symmetry properties of  $B(\omega, \xi, \xi')$ :

$$(8.3) \quad B(\omega, \xi, \xi') = B(\omega, \xi', \xi) = B(\omega, \xi_\star, \xi'_\star).$$

Clearly, the integral in (8.2) is zero (independent of  $f$ ) if  $\phi + \phi' = \phi_\star + \phi'_\star$ . It is well-known [2] that

$$(8.4) \quad \phi + \phi' = \phi_\star + \phi'_\star \quad \text{if and only if} \quad \phi(\xi) \in \text{span}\{1, \xi_1, \xi_2, \dots, \xi_d, |\xi|^2\}.$$

Moment closure systems considered here are derived from the Boltzmann equation as follows. Let  $n$  be a positive integer and give  $n$  linearly independent continuous functions  $c_k = c_k(\xi)$  of  $\xi \in \mathbf{R}^d$  ( $k = 1, 2, \dots, n$ ). Multiplying (8.1) with  $c_k(\xi)$  and integrating the resulting equations with respect to  $\xi \in \mathbf{R}^d$  leads to  $n$  equations

$$(8.5) \quad \partial_t \int c_k f d\xi + \nabla_x \cdot \int \xi c_k f d\xi = \int c_k (f_\star f'_\star - f f') B d\omega d\xi' d\xi.$$

Let  $\alpha_k = \alpha_k(x, t)$  ( $k = 1, 2, \dots, n$ ) be  $n$  unknown scalar functions of  $(x, t)$ . Substituting

$$(8.6) \quad f = f(x, t, \xi) = \exp\left(\sum_{k=1}^n c_k(\xi) \alpha_k(x, t)\right)$$

into (8.5), we get  $n$  first-order PDEs for the  $n$  unknown  $\alpha_k$ .

*Remark 8.1.* Traditionally, each  $c_k$  is a polynomial of  $\xi$  and  $\int c_k f d\xi$  is called a *moment*. Here we do not require the  $c_k$ 's to be polynomials.

To make clear that the moment closure systems in (8.5) with (8.6) are of the form (1.1), we write  $c(\xi)\alpha = \sum_{k=1}^n c_k(\xi)\alpha_k$  and introduce the following functions of  $\alpha \in \mathbf{R}^n$ :

$$(8.7) \quad \begin{aligned} \bar{\eta}(\alpha) &= \int \exp(c(\xi)\alpha) d\xi, \\ q_j(\alpha) &= \int \xi_j \exp(c(\xi)\alpha) d\xi, \\ \mathcal{Q}(\alpha) &= \begin{pmatrix} \mathcal{Q}_1 \\ \mathcal{Q}_2 \\ \vdots \\ \mathcal{Q}_n \end{pmatrix} = \int \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix} (\exp(c_\star \alpha + c'_\star \alpha) - \exp(c' \alpha + c \alpha)) B d\omega d\xi' d\xi. \end{aligned}$$

Here we have considered

$$(8.8) \quad f_\star f'_\star = \exp(c_\star \alpha + c'_\star \alpha) \quad \text{and} \quad f f' = \exp(c \alpha + c' \alpha)$$

thanks to the Ansatz in (8.6). With such an  $f$ , we formally have

$$\bar{\eta}_{\alpha_k} \equiv \frac{\partial \bar{\eta}}{\partial \alpha_k} = \int c_k f d\xi \quad \text{and} \quad q_{j\alpha_k} \equiv \frac{\partial q_j}{\partial \alpha_k} = \int \xi_j c_k f d\xi.$$

Thus (8.5) can be rewritten as

$$(8.9) \quad \frac{\partial \bar{\eta}_\alpha(\alpha)}{\partial t} + \sum_j \frac{\partial q_{j\alpha}(\alpha)}{\partial x_j} = \mathcal{Q}(\alpha).$$

Assume that there is a convex open set  $\mathcal{G} \subset \mathbf{R}^n$  such that the functions in (8.7) are well-defined and smooth for  $\alpha \in \mathcal{G}$ . The existence of such a  $\mathcal{G}$  depends on the choice of the  $c_k$ 's and will not be addressed here. The interested reader is referred to [15].

Define

$$U = \bar{\eta}_\alpha(\alpha) \quad \text{and} \quad G = \bar{\eta}_\alpha(\mathcal{G}).$$

We show that, for any  $U \in G$ , there is a unique  $\alpha \in \mathcal{G}$  such that  $U = \bar{\eta}_\alpha(\alpha)$ . In fact, since the  $c_k$ 's are linearly independent, the Hessian matrix  $\bar{\eta}_{\alpha\alpha}(\alpha)$  is symmetric positive definite and thereby  $\bar{\eta}(\alpha)$  is strictly convex. Then the strictly convex function  $(\bar{\eta}(\alpha) - \alpha^*U)$  of  $\alpha \in \mathcal{G}$  takes its local minimum at those  $\alpha$  satisfying  $U = \bar{\eta}_\alpha(\alpha)$ . Since  $\mathcal{G}$  is convex, there is at most one such minimum point. Consequently,  $U = \bar{\eta}_\alpha(\alpha)$  has a global inverse  $\alpha = \alpha(U)$  for  $U \in G$  and  $G$  is diffeomorphic to the convex open set  $\mathcal{G}$ .

For  $U \in G$ , set

$$\eta(U) := \alpha^*(U)U - \bar{\eta}(\alpha(U)).$$

We see that the inverse function  $\alpha(U)$  is equal to  $\eta_U(U)$ . Thus, with

$$(8.10) \quad F_j(U) := q_{j\alpha}(\eta_U(U)) \quad \text{and} \quad Q(U) := \mathcal{Q}(\eta_U(U)),$$

we arrive at the following system of PDEs:

$$(8.11) \quad \frac{\partial U}{\partial t} + \sum_j \frac{\partial F_j(U)}{\partial x_j} = Q(U).$$

In [15], Levermore showed that  $\eta(U)$  defined above is a strictly convex entropy function for (8.11) in the classical sense (I).

To verify the observed properties (II) and (III), we use (8.2) and rewrite  $\mathcal{Q}(\alpha)$  defined in (8.7) as

$$\mathcal{Q}(\alpha) = \frac{-1}{4} \int \begin{pmatrix} c_{1*} + c'_{1*} - c'_1 - c_1 \\ c_{2*} + c'_{2*} - c'_2 - c_2 \\ \vdots \\ c_{n*} + c'_{n*} - c'_n - c_n \end{pmatrix} (\exp(c_*\alpha + c'_*\alpha) - \exp(c'\alpha + c\alpha)) B d\omega d\xi' d\xi.$$

Notice that

$$\begin{aligned} & \exp(c_*\alpha + c'_*\alpha) - \exp(c'\alpha + c\alpha) \\ &= \int_0^1 \exp[\sigma(c_* + c'_* - c' - c)\alpha + (c' + c)\alpha] d\sigma (c_* + c'_* - c' - c)\alpha. \end{aligned}$$

We set

$$b = b(\alpha, \xi, \xi', \xi'_*, \xi_*) = \int_0^1 \exp[\sigma(c_* + c'_* - c' - c)\alpha + (c' + c)\alpha] d\sigma$$

and define

$$(8.12) \quad a_{ij}(\alpha) = \frac{1}{4} \int (c_{i*} + c'_{i*} - c'_i - c_i) b B (c_{j*} + c'_{j*} - c'_j - c_j) d\omega d\xi' d\xi.$$

Thus,  $\mathcal{L}(U) = [a_{ij}(\eta_U(U))]_{n \times n}$  is a symmetric matrix and

$$Q(U) = \mathcal{Q}(\eta_U(U)) = -\mathcal{L}(U)\eta_U(U).$$

Since  $b$  and  $B$  are both positive, it follows from (8.12) that  $\mathcal{L}(U)$  is non-negative. Moreover, the null space of  $\mathcal{L}(U)$  is

$$\left\{ \alpha \in \mathbf{R}^n : \int |(c(\xi) + c(\xi') - c(\xi_*) - c(\xi'_*))\alpha|^2 d\omega d\xi d\xi' = 0 \right\},$$

which is independent of  $U$ . Hence the observation holds for the moment closure systems in [15].

## 9. DISCRETE VELOCITY MODELS

In this section, we consider discrete velocity models in kinetic theories [7]:

$$(9.1) \quad f_{kt} + a(k) \cdot \nabla_x f_k = Q_k(U)$$

for  $k = 1, 2, \dots, n$ . Here  $f_k = f_k(x, t)$  denotes the mass density of gas particles with the constant velocity  $a(k) \in \mathbf{R}^d$  at time  $t$  and position  $x$ ,  $a(k) \cdot \nabla_x = \sum_{j=1}^d a_j(k) \partial_{x_j}$ ,  $U = (f_1, f_2, \dots, f_n)^*$ , and  $Q_k(U)$  is the collision term given by

$$(9.2) \quad Q_k(U) = \sum_{ijl} (A_{ij}^{kl} f_i f_j - A_{kl}^{ij} f_k f_l),$$

where the summation is taken over all  $i, j, l \in \{1, 2, \dots, n\}$  and the coefficients  $A_{ij}^{kl}$  are non-negative constants satisfying

$$(9.3) \quad A_{ij}^{kl} = A_{kl}^{ij} = A_{lk}^{ij}.$$

It is not difficult to deduce from these symmetry properties that

$$(9.4) \quad \sum_{k=1}^n \phi_k Q_k(U) = \frac{1}{4} \sum_{ijkl} A_{ij}^{kl} (\phi_k + \phi_l - \phi_i - \phi_j) (f_i f_j - f_k f_l)$$

Remark that (9.3) and (9.4) are analogous to the fundamental properties in (8.3) and (8.2) of the Boltzmann equation.

Our aim here is to show that, in the state space

$$G := \{f_k > 0 : k = 1, 2, \dots, n\} \ni U,$$

the discrete velocity model (9.1)-(9.3) admits our observation with the strictly convex function

$$(9.5) \quad \eta(U) = \sum_{k=1}^n f_k (\log f_k - 1).$$

The strict convexity of  $\eta(U)$  is obvious. Since it does not contain any cross-term,  $\eta(U)$  is an entropy function for the diagonal and semilinear system (9.1).

To see the properties (II) and (III), we set

$$b_{ij}^{kl} = b_{ij}^{kl}(U) = \int_0^1 \exp[\sigma(\log f_i + \log f_j - \log f_k - \log f_l) + \log f_k + \log f_l] d\sigma > 0,$$

which obviously has the symmetry properties (9.3). Then the source terms can be rewritten as

$$(9.6) \quad \begin{aligned} Q_k(U) &= \sum_{ijl} A_{ij}^{kl} b_{ij}^{kl} (\log f_i + \log f_j - \log f_k - \log f_l) \\ &= - \sum_m a_{km} \log f_m, \end{aligned}$$

where

$$a_{km}(U) = - \sum_{jl} A_{mj}^{kl} b_{mj}^{kl} - \sum_{il} A_{im}^{kl} b_{im}^{kl} + \sum_{ij} A_{ij}^{km} b_{ij}^{km} + \delta_{km} \sum_{ijl} A_{ij}^{kl} b_{ij}^{kl}$$

with  $\delta_{km}$  the Kronecker delta. Therefore, we have

$$(9.7) \quad Q(U) = -[a_{km}]_{n \times n} \eta_U(U) \equiv -\mathcal{L}(U) \eta_U(U),$$

for  $\eta_U(U) = (\log f_1, \log f_2, \dots, \log f_n)^*$  due to (9.5).

It remains to check the desired properties of  $\mathcal{L}(U)$  defined in (9.7). Thanks to the symmetry properties (9.3) for both  $b_{ij}^{kl}$  and  $A_{ij}^{kl}$ , it is not difficult to see that  $a_{km} = a_{mk}$ , that is,  $\mathcal{L}(U)$  is symmetric. Moreover, let  $y = (y_1, y_2, \dots, y_n) \in \mathbf{R}^n$ . We refer to (9.4) and (9.6) to obtain

$$y \mathcal{L}(U) y^* = \frac{1}{4} \sum_{ijkl} A_{ij}^{kl} b_{ij}^{kl} (y_i + y_j - y_k - y_l)^2 \geq 0.$$

Hence,  $\mathcal{L}(U)$  is non-negative and its null space is

$$\{y \in \mathbf{R}^n : A_{ij}^{kl} (y_i + y_j - y_k - y_l) = 0 \text{ for all } i, j, k, l\}.$$

which is independent of  $U$ . Hence, our observation holds for the discrete velocity kinetic models constructed in [7].

We conclude this paper by writing down the simplified system (3.2) for the discrete velocity models. To do this, we compute from (9.5) that  $\eta_U(U) = (\log f_1, \log f_2, \dots, \log f_n)^*$ . Then the corresponding simplified system reads as

$$\begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix}_t + \sum_j \begin{pmatrix} a_j(1) & 0 & \cdots & 0 \\ 0 & a_j(2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_j(n) \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix}_{x_j} = -\mathcal{L} \begin{pmatrix} \log f_1 \\ \log f_2 \\ \vdots \\ \log f_n \end{pmatrix}$$

where  $\mathcal{L}$  is a constant, symmetric and non-negative definite  $n \times n$ -matrix.

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